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Reference Manual for the KfK Code PCROSS

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Referenzhandbuch für das KfK Programm PCROSS

Kurzfassung

Das Programm PCROSS berechnet sogenannte "Pseudo"- Wirkungsquerschnitte für sequentielle (x,n) -Reaktionen und vereinigt diese mit den effektiven Wirkungsquerschnitten von neutroneninduzierten Reaktionen zu einem über das Spektrum integrierten Datensatz. Dieser dient als modifizierter Eingabedatensatz für das Programm FISPACT, das die Aktivierung und abgeleitete radiologische Eigenschaften von Materialien berechnet, die in einem definierten Neutronenfeld bestrahlt werden. Der vorliegende Bericht gibt eine Kurzbeschreibung des zugrundeliegenden Algorithmus und enthält die wesentlichen technischen Details des Programms PCROSS (Version 1.0) sowie die Beschreibungen der Parameter, der Common-Blöcke und der Unterprogramme.

Abstract

The PCROSS code calculates the so-called "pseudo" cross sections for sequential (x,n) reactions and merges them together with "effective" cross sections for neutron induced reactions into one file of "collapsed" cross sections. The file is tailored to provide an input for the FISPACT inventory code that calculates the activation and related radiological quantities of material irradiated in given neutron fields. The present report summarizes calculational procedure and provides the reader with essential technical details of the code PCROSS (version 1.0) such as description of parameters, common blocks and subroutines.

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1. INTRODUCTION

The importance of sequential (x,n) reactions in fusion materials activation calculations, x being light charged particles created by primary neutron interactions, has been demonstrated recently [1, 2]. This triggered a concentrated effort to study such contributions on a systematic basis. First, the corresponding nuclear data base has been developed [3]. Second, the KfK code PCROSS [4] has been developed that uses this data base and calculates key intermediary quantities, so-called "pseudo" cross sections for sequential (x,n) reactions. PCROSS merges these cross sections together with "collapsed" cross sections for primary neutron-induced reactions into one file tailored to provide an input for the well established FISPACT inventory code that calculates activation of material irradiated in a neutron flux [5, 6].

The user manual for the code PCROSS is described elsewhere [4]. The aim of the present report is to supplement it and to provide the reader with basic technical details of the code (version 1.0) such as description of parameters, common blocks and subroutines.

2. CALCULATIONAL PROCEDURE

The nuclear data base needed for a systematic inclusion of sequential (x,n) reactions into inventory calculations is described in Ref.[3]. Apart from the evaluated file REAC-ECN-5¹ for (n,x) cross sections [7], the base has three major KfK libraries: KFKSPEC for normalized (n,x) spectra, KFKXN for (x,n) cross sections, and KFKSTOP for differential ranges of light charged particles. The calculational procedure adopted in PCROSS uses all these libraries and proceeds as follows:

For a given initial composition of a fusion reactor material, which can be composed by using several Input Data Cards (see user manual of the code PCROSS [4]) and for a given neutron field one calculates a flux of charged particles of the type x, where $x = p, d, t, {}^3He$ and α . The charged particle flux from single isotopes/elements is added up to create a total charged particle flux for the initial elemental composition. This flux is then used to evaluate averaged cross sections for (x,n) reactions on all stable as well as radioactive isotopes included in any actual FISPACT input list. These cross sections known as "pseudo" cross sections are fully defined in [3]. They can be used in inventory

¹The file REAC-ECN-5 is identical with the European Activation File EAF-1. We use the older name for this file throughout this report to maintain the consistency with our previous two reports of this series [3, 4].

calculations exactly in the same manner as the usual "collapsed" cross sections for neutron induced reactions. "Collapsed" cross sections are usually calculated with the FISPACT program using the COLLAPSE option (see Fig.1). We merge "effective" cross sections together with "pseudo" cross sections to create a unique input file of "collapsed" cross sections for the inventory code FISPACT (see Fig.2).

For convenience we repeat here some basic definitions as introduced in [3]. In the description section of common blocks and of subroutines we will furthermore refer to the quantities defined below. The flux $\Phi_x(E_{x_k})$ ($cm^{-2}s^{-1}$) of charged particles x with the energy E_{x_k} created by neutrons incident on a material composed of various stable isotopes A is defined as

$$\Phi_x(E_{x_k}) = \sum_A \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \sum_{j=k}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \Delta R_x(E_{x_k}). \quad (1)$$

Here, $\Phi_n(E_{n_i})$ ($cm^{-2}s^{-1}u^{-1}$) is the neutron flux in the i -th energy interval of the fusion spectrum, ΔE_{n_i} (u) refers to the neutron lethargy energy bin as also used in the REAC-ECN-5 library, $\sigma_{n,x}(E_{n_i})$ (cm^2) is the production cross section of charged particle x in the neutron energy group E_{n_i} , and N_A (cm^{-3}) is the number of atoms of the initial nuclide A . Next, $f_{n,x}(E_{n_i}, E_{x_j})$ (MeV^{-1}) represents the normalized charged particle spectrum from the reaction $A(n, x)$ given in uniform energy steps of $\Delta E_{x_j} = 1 MeV$ and referring to the i -th incident neutron energy group, the charged particle energy being $E_{x_j} = 0.5, 1.5, \dots, 23.5 MeV$. Finally, $\Delta R_x(E_{x_k})$ (cm) is the differential thickness of the surrounding material corresponding to 1 MeV step of energy loss of charged particles with the starting energy E_{x_k} . The "pseudo" cross section $\sigma_{x,C}^{pseudo}$ (cm^2) for the sequential reaction $\bar{A}(x, n)C$, where \bar{A} can be any isotope we are interested in, is then defined as

$$\sigma_{x,C}^{pseudo} = \frac{1}{\sum_{i=1}^{175} \Phi_n(E_{n_i}) \Delta E_{n_i}} \sum_{k=1}^{24} \Phi_x(E_{x_k}) \sigma_{x,C}(E_{x_k}). \quad (2)$$

Here, $\sigma_{x,C}(E_{x_k})$ (cm^2) stands for the production cross section of the nucleus C via the sequential reaction $\bar{A}(x, n)C$. The "pseudo" cross section is given per one initial neutron rather than per one charged particle, hence its name.

The quantities $\sigma_{n,x}$ are derived from the library REAC-ECN-5, normalized spectra $f(n, x)$ are taken from the KFKSPEC, differential ranges ΔR_x are from the KFKSTOP, and production cross sections $\sigma_{x,C}$ are from the library KFKXN.

3. PARAMETERS AND COMMON BLOCKS

3.1. Parameters

Below we describe all parameters used in the code PCROSS. The parameters determine the size of arrays used in common blocks, the range of DO-loops and the I/O units. We reproduce the parameter statement given in the code to show the actual values of parameters. This is followed by the definitions of the individual parameters.

```

PARAMETER (LFIS =1315,LELE = 92,LISO = 640,LCAL =3500,
&          LNXR = 5,LXNR = 10,LXGR = 24,LNGR = 20,
&          LNAL = 50,LNNM = 175,LIN1 = 21,LIN2 = 22,
&          LIN3 = 23,LIN5 = 25,LIN7 = 27,
&          LIN10= 41,LIN11= 42,LIN12= 43,LIN13= 44,
&          LIN14= 45,LIN20= 51,LIN21= 52,LIN22= 53,
&          LIN23= 54,LIN24= 55,LIN25= 56,LIN26= 57,
&          LOUT = 31,LRES = 32)

```

Definitions:

- **LFIS** is the number of isotopes mentioned in the isotope index file of FISPACT. This file is called ACT10P.INDEX in Ref.[4].
- **LELE** is the number of all elements from hydrogen up to uranium.
- **LISO** is the maximum number of isotopes to be calculated.
- **LCAL** is the maximum number of sequential (x,n) reactions to be calculated.
- **LNXR** is the number of different types of charged particle x in (n,x) reactions. Current types are $x = p, d, t, {}^3He$ and α .
- **LXNR** is the number of different (x,n) reaction types and different (x,2n) reaction types, x are the same particles as already mentioned above.
- **LXGR** is the number of 1 MeV bins used for the energy grouping of outgoing charged particles from (n,x) reactions. The charged particle energies are $E_{x_j} = 0.5, 1.5, \dots, 23.5$ MeV. The parameter LXGR is also used to dimension the field of $\Delta R_x(E_{x_k})$ which is the differential thickness of the surrounding material for 1 MeV energy loss of charged particles with the starting energy E_{x_k} , and the field of $\sigma_{x,c}(E_{x_k})$ which is the production cross section of the nucleus C via the sequential reaction $\bar{A}(x, n)C$.
- **LNGR** is the number of bins we use to regroup the lethargy groups of the neutron energies of $\Phi_n(E_{n_i})$ in the normalized charged particle spectrum $f_{n,x}(E_{n_i}, E_{x_j})$. LNGR energy groups of E_{n_i} are used to match the hole range of 175 groups of the VITAMIN-J structure.
- **LNAL** is the maximum number of elements composing an alloy.
- **LNNM** is the number of bins to group the initial neutron flux $\Phi_n(E_{n_i})$ into lethargy groups according to the VITAMIN-J structure.
- **LIN1** is the input unit connected to the file with the initial neutron flux $\Phi_n(E_{n_i})$.
- **LIN2** is the input unit connected to the REAC-ECN-5 file, where all cross sections $\sigma_{n,x}(E_{n_i})$ are listed.

- LIN3 is the input unit connected to the file containing collapsed cross sections of all neutron induced reactions (n,x) as calculated by FISPACT for a given neutron spectrum.
- LIN5 is the input unit connected with the KFKSPEC library. This file contains the quantities $f_{n,x}(E_{n_i}, E_{x_j})$ (MeV^{-1}), which represent the normalized charged particle spectrum for each isotope and each type of charged particle.
- LIN7 is the input unit connected with the ACT10P.INDEX file. This file gives the indices in the FISPACT notation as well as in the EEEIIM notation where EEE stands for the element identifier, III for the isotope identifier and M indicates a possible isomeric state.
- LIN10, LIN11, LIN12, LIN13, LIN14 are the input units connected to the energy range files for p, d, α , t, 3He of the KFKSTOP library, respectively.
- LIN20, LIN21, LIN22, LIN23, LIN24, LIN25, LIN26 are the input units connected to the (p, n), (d, n), (α , n), (t, n), (3He , n) as well as (d, 2n), (t, 2n) cross section files of the KFKXN library, respectively.
- LOUT is the output unit for calculated "pseudo" cross sections listed in a sequence and associated with the FISPACT isotope identifiers.
- LRES is the output unit connected to the file containing the above "pseudo" cross sections merged together with the "collapsed" cross sections obtained from the unit LIN3. All these cross sections are accompanied with the FISPACT isotope identifiers and used as a modified input file for the FISPACT inventory calculation.

3.2. Common blocks

In this section we describe common blocks as used by the code PCROSS. We reproduce full COMMON statements, give definitions of variables and list subroutines that have an access to the common block under discussion.

3.2.1. Common block CPARTS

```
COMMON/CPARTS/CPSPP(LXGR,LNGR),CSPD(LXGR,LNGR),CSPA(LXGR,LNGR),  
&           CPSPT(LXGR,LNGR),CSPH(LXGR,LNGR)  
REAL CPSPP,CSPD,CSPA,CPSPT,CSPH
```

Definitions:

- CPSPP is the field which contains the normalized proton spectrum $f_{n,p}(E_{n_i}, E_{p_j})$ (MeV^{-1}) from the reaction $A(n,p)$ given in uniform energy steps of $\Delta E_{p_j} = 1MeV$.
- CSPD, CSPA, CPSPT, CSPH are fields similar to CPSPP containing the normalized charged particle spectra of d, α , t and 3He particles, respectively.

Access:

The common block CPARTS is used by the following subroutines:
PCGCPS, PCPRES.

3.2.2. Common block CPSCDC

```
COMMON/CPSCDC/IINIT(LCAL), IORGN(LCAL), IFINL(LCAL), IREAC(LCAL),  
&                CPSCD(LCAL), IISO1(LCAL), IISO2(LCAL), ICOUNT  
REAL    CPSCD  
INTEGER IINIT, IORGN, IFINL, IREAC, IISO1, IISO2, ICOUNT
```

Definitions:

- **IINIT** is the integer field containing the identifier of the nucleus A in a given sequential reaction. This identifier is the same as used by FISPACT (see also our file ACT10P.INDEX). The full description of the reaction as well as the value of the "pseudo" cross section are stored under the same indices in other fields of this common block.
- **IORGN** is the integer field containing the identifier of the nucleus \bar{A} in a given sequential reaction. The identifiers used are the same as in the field IINIT.
- **IFINL** is the integer field containing the identifier of the nucleus C in a given sequential reaction. The identifiers used are the same as in the field IINIT.
- **IREAC** is the field that shows the type of the (x,n) reaction of the sequential reaction.
- **CPSCD** is the field containing "pseudo" cross sections $\sigma_{x,C}^{pseudo}$.
- **IISO1** is the integer field that contains the identifier of the nucleus \bar{A} in a given sequential reaction. The identifiers used are of the type EEEIIM, where EEE stands for the element identifier, II for the isotope identifier and M indicates possible isomeric states of the nuclide \bar{A} .
- **IISO2** is the integer field that contains the identifier of the nucleus C in a given sequential reaction. The identifiers used are of the type EEEIIM.
- **ICOUNT** is the number of calculated sequential reactions.

Access:

The common block CPSCDC is used by the following subroutines:
PCLOOP, PCMERG.

3.2.3. Common block CVALUE

```
COMMON/CVALUE/CCNX(LNNM), DEX(LXGR), DNX(LXGR, LNGR),  
&                CXN(LXGR), SUMCPS(LXGR, LNXR),  
&                VCN, ABD, RO, PSDC  
REAL CCNX, DEX, DNX, CXN, VCN, ABD, RO, PSDC, SUMCPS
```

We note that the values of all variables as well as arrays in this common block are permanently updated for every isotope and for every reaction type under calculation.

Definitions:

- **CCNX** contains the cross section $\sigma_{n,x}(E_{n_i})$ (barns). This is the production cross section of charged particle x in the neutron energy group E_{n_i} . Note that CCNX is just valid for the actual type of the charged particle x .

- **DEX** is the field containing $\Delta R_x(E_{x_k})$ (*cm*) which is the differential thickness of the surrounding material corresponding to 1 MeV step of the energy loss of charged particles x with the starting energy E_{x_k} . The type of the charged particle x is the same as for the field CCNX.
- **DNX** is the field which contains the normalized charged particle spectrum $f_{n,x}(E_{n_i}, E_{x_j})$ (MeV^{-1}) from the reaction $A(n, x)$ given in uniform energy steps of $\Delta E_{x_j} = 1MeV$. The type of the charged particle x is the same as in the fields mentioned above.
- **CXN** contains the (x,n) cross section $\sigma_{x,C}(E_{x_k})$ (*barns*) which stands for the production cross section of the nucleus C via the sequential reaction $\bar{A}(x, n)C$. The type of the charged particle x is the same as in the fields mentioned above.
- **SUMCPS** is the field containing the flux $\Phi_x(E_{x_k})$ ($cm^{-2}s^{-1}$) of charged particles x with the energy E_{x_k} created by neutrons incident on a material composed of various stable isotopes A . The field SUMCPS is handling the flux of p, d, α, t and 3He particles in separate subfields.
- **VCN** is the number of atoms (*at/cm³*) of the initial nuclide A in a natural composition of the corresponding single element.
- **ABD** is the natural abundancy of the isotope A in its own element.
- **RO** is the density (*g/cm³*) of the element in its natural composition. The density for the isotope A is identical for all isotopes of the same element.
- **PSDC** is the "pseudo" cross section calculated for the sequential reaction $\bar{A}(x, n)C$.

Access:

The common block CVALUE is used by the following subroutines:
PCCALC, PCCALS, PCGECO, PCLOOP, PCPRES, PCRESC, PCRESP.

3.2.4. Common block DFLUXS

```
COMMON/DFLUXS/DELTA(LNNM), ILETHA(LNNM)
REAL DELTAF
INTEGER ILETHA
```

Definitions:

- **DELTA** refers to the neutron lethargy energy bin in units (u) and it is set to $\Delta E_{n_i} = 1.0$.
- **ILETHA** is the integer field that indicates which of the neutron energy bins of $\Phi_n(E_{n_i})$ we use for the neutron energies in the normalized charged particle spectrum $f_{n,x}(E_{n_i}, E_{x_j})$.

Access:

The common block DFLUXS is initiated by the BLOCK DATA and used by the following sub-routine:
PCCALS.

3.2.5. Common block ECONST

```
COMMON/ECONST/CIAB(LISO), CIAW(LISO), CIRO(LISO), ICPN(LISO)
REAL CIAB, CIAW, CIRO
INTEGER ICPN
```

Definitions:

- **CIAB** contains the natural abundancy of all stable and radioactive isotopes with $T_{1/2} > 1d$ which are listed in the material index file ACT10P.INDEX.
- **CIAW** contains the atomic weight of elements in their natural composition. The atomic weight for the isotope is identical for all isotopes of the same element.
- **CIRO** contains the density in units of (g/cm^3) of elements in their natural composition. The density for the isotope is identical for all isotopes of the same element.
- **ICPN** contains isotope identifiers of isotopes listed in the arrays described above. The form of the identifier is EEEIIM.

Access:

The common block **ECONST** is initiated by the BLOCK DATA and used by the following sub-routines:

PCGECO, PCLOOP.

3.2.6. Common block IDENTI

COMMON/IDENTI/IREACM(LNXR),IXCPNT(LXNR),ISPPNT(LNXR),IFINAL(LXNR),
& CALVEC(LISO),ICALPT,ICALRM
INTEGER IREACM,IXCPNT,ISPPNT,IFINAL,CALVEC,ICALPT,ICALRM

Definitions:

- **IREACM** is the field of reaction identifiers. Reactions (n,p) , (n,d) , (n,t) , $(n,^3He)$, (n,α) are identified by the number 1030, 1040, 1050, 1060, 1070, respectively.
- **IXCPNT** is the field of pointers for cross sections $\sigma_{x,C}(E_{x_k})$ in the common block XNCROS. In this field the reaction types are ordered as (p,n) , (d,n) , (t,n) , $(^3He,n)$, (α,n) and these are followed by $(p,2n)$, $(d,2n)$, $(t,2n)$, $(^3He,2n)$, $(\alpha,2n)$. However, only $(d,2n)$ and $(t,2n)$ cross sections are currently available from the library KFKXN.
- **ISPPNT** is the field of pointers for the differential thickness of the surrounding material, $\Delta R_x(E_{x_k})$ (cm), in the common block STOPPS. In this field the types of charged particles x are ordered as p , d , t , 3He , α .
- **IFINAL** is the integer field that contains the identifier of the nucleus C in a given sequential reaction. The identifiers used are the same as in the isotope index file used by FISPACT. Different final nuclides C are stored for different types of (x,n) reactions for the same nucleus \bar{A} in the reaction $\bar{A}(x,n)C$.
- **CALVEC** is the integer field which contains all possible nuclides \bar{A} for which "pseudo" cross sections will be calculated.
- **ICALPT** is the pointer to the current nuclide out of various nuclides \bar{A} in the CALVEC field.
- **ICALRM** indicates the charged particle reaction type.

Access:

The common block **IDENTI** is initiated by the BLOCK DATA and used by the following sub-routines:

PCCALC, PCCALS, PCGCXN, PCGSTP, PCLOOP, PCPRES, PCRESA.

3.2.7. Common block IFISDI

```
COMMON/IFISDI/IDFIS(LFIS),IDDSC(LFIS)
INTEGER      IDFIS,IDDSC
```

Definitions:

- **IDFIS** is the integer field containing the FISPACT identifiers for isotopes.
- **IDDSC** is the integer field that corresponds to the above field IDFIS but the identifier of an isotope has the notation EEEIIM.

Access:

The common block **IFISDI** is used by the following subroutines:
PCLOOP, PCREAD.

3.2.8. Common block LSTEER

```
COMMON/LSTEER/COLVEC(LNAL),COLABD(LNAL),ICROSS,
&          LCTOTA,LMERGE,LCCROS,LALLOY
REAL      COLABD
INTEGER   COLVEC,ICROSS
LOGICAL   LCTOTA,LMERGE,LCCROS,LALLOY
```

Definitions:

- **COLVEC** is the integer field containing all element identifiers that are components of an alloy. COLVEC is used only for a calculation with the "ALLY" input card, see Ref.[4].
- **COLABD** is the real field containing relative weights of elements in the alloy. COLABD is used only for a calculation with the "ALLY" input card, see Ref.[4].
- **ICROSS** is the variable declaring how many neighbouring elements *m* are taken into account to calculate "pseudo" cross sections in the case when the "ELEP *m*" input card is used, see Ref.[4].
- **LCTOTA** is the logical variable indicating calculation with the "ELEP 0" input card, see Ref.[4].
- **LMERGE** is the logical variable indicating that the calculated "pseudo" cross section has to be merged into the FISPACT file containing "collapsed" cross sections.
- **LCCROS** is the logical variable declaring that neighbouring element has to be taken into account in the case of a calculation with the "ELEP *m*" input card, see [4].
- **LALLOY** is the logical variable declaring that the initial composition is an alloy and that the components of this alloy will be listed in the field COLVEC.

Access:

The common block **LSTEER** is used by the subroutines:
PCGCNX, PCGSTP, PCLOOP, PCMERG, PCRDU5, PCRESA.

3.2.9. Common block PCCTRL

```
COMMON/PCCTRL/LFOUND,LCPSKP,LCPSKH,LDEBUG,LBEGIN,LONCES,  
&              LALCU(LNXR),LCALIS(LXNR),LWROUT,LCOLVC,LCOLEL,  
&              LCALSP  
LOGICAL LFOUND,LCPSKP,LCPSKH,LDEBUG,LBEGIN,LONCES,LALCU,  
&              LCALIS,LWROUT,LCOLVC,LCOLEL,LCALSP
```

Definitions:

- **LFOUND** is the global logical variable pointing out whether an attempt to find required data in a library was successful or not.
- **LCPSKP** is the logical variable indicating that the information about cross sections $\sigma_{n,x}(E_{n_i})$ for a nucleus A was found in the REAC-ECN-5 library, but the identifier for the data about normalized charged particle spectra $f_{n,x}(E_{n_i}, E_{x_j})$ in the library KFKSPEC was too high. The identifier used for comparison is stored in the common block PCIDIS.
- **LCPSKH** is the logical variable indicating that the information about the cross sections $\sigma_{n,x}(E_{n_i})$ for a nucleus A was found in the REAC-ECN-5 library, but the identifier of the nucleus coming up from the KFKSPEC library when reading in $f_{n,x}(E_{n_i}, E_{x_j})$ was too low. The identifier used for comparison is stored in the common block PCIDIS.
- **LDEBUG** is used for debugging purposes only.
- **LBEGIN** is the logical variable that indicates that the program is starting up with the first read-in from the REAC-ECN-5 file.
- **LONCES** is the logical variable indicating that the program reads-in cross sections from the REAC-ECN-5 file for a nucleus A that belongs to the same element as the cross sections in the previous loop.
- **LALCU** is the field of logical variables which control allowed reactions. When the program detects, that a part of data needed to calculate a contribution to the charged particle flux from the reaction $A(n, x)$ is missing, the calculation of the affected reaction will be suppressed.
- **LCALIS** is the field of logical variables which control allowed sequential reactions. When the program detects, that a part of data needed to calculate the "pseudo" cross section in the reaction $\bar{A}(x, n)C$ or $\bar{A}(x, 2n)C$ is missing, the calculation of the affected reaction will be suppressed.
- **LWROUT** is the logical variable indicating whether information for a given nucleus should be printed out.
- **LCOLVC** is the logical variable indicating whether the isotope, for which the program is getting data, is a component of an alloy.
- **LCOLEL** is the logical variable controlling that the build up of the charged particle flux $\Phi_x(E_{x_k})$ has been completed. This refers to the case when the initial composition of material is limited to a single element.
- **LCALSP** is the logical variable indicating whether the query for $\Delta R_x(E_{x_k})$ of an element was successful.

Access:

The common block PCCTRL is used by the following subroutines:

PCGCPS, PCGCXN, PCGECO, PCGSTP, PCLOOP, PCPRES, PCRESA, PCRESC, PCGCNX.

3.2.10. Common block PCIDIS

```
COMMON/PCIDIS/IDNOW, IDNEW, ICIOS, IDCPAI
INTEGER IDNOW, IDNEW, ICIOS, IDCPAI
```

Definitions:

- **IDNOW** is used to store the isotope identifier of the nucleus A. It stands for the nucleus A in the reaction $A(n, x)$. It is the identifier of the nucleus in the description of the REAC-ECN-5 file.
- **IDNEW** is used to store the isotope identifier of the nucleus A which follows the identifier stored in IDNOW. This identifier describes the next (n,x) reaction in the REAC-ECN-5 file.
- **IDCPAI** is used to store the isotope identifier of the nucleus A in the KFKSPEC file. It is read-in from the header of the charged particle spectrum and used for comparison with IDNOW. In this way, the program looks for coincident appearance of the same identifiers in both variables in order to proceed with the calculation of the "pseudo" cross section.
- **ICIOS** is the isotope number III of the nucleus A stored in IDNOW with the identifier of the type EEEIIM.

Access:

The common block **PCIDIS** is used by the following subroutines:
PCGCNX, PCGCPS, PCGECO, PCGSTP, PCLOOP, PCRESA.

3.2.11. Common block PCSTOP

```
COMMON/PCSTOP/STOPPC
LOGICAL STOPPC
```

Definitions:

- **STOPPC** is the logical variable indicating that the program PCROSS will terminate.

Access:

The common block **PCSTOP** is used by the following subroutines:
PCGCNX, PCGCPS, PCLOOP.

3.2.12. Common block P NAMES

```
COMMON/P NAMES/NAME(104), NAMREP(104)
CHARACTER*4 NAME, NAMREP
```

Definitions:

- **NAME** is the character field containing chemical symbols of elements in mixed letters.
- **NAMREP** is the character field containing chemical symbols of elements in capital letters.

Access:

The common block **P NAMES** is initiated by the **BLOCK DATA** and it is used by the following subroutines:
PCGCNX, PCGSTP, PCLOOP, PCMERG, PCRDU5, PCGCPS.

3.2.13. Common block NEUTRN

```
COMMON/NEUTRN/VITJ(LNNM+1)
REAL VITJ
```

Definitions:

- VITJ is the field containing the energy boundaries of the LNNM group structure for the neutron flux $\Phi_n(E_{n_i})$, and the production cross section $\sigma_{n,x}(E_{n_i})$ of the charged particle x.

Access:

The common block NEUTRN is initiated by the BLOCK DATA and it is used by the following subroutine:

— .

3.2.14. Common block NXCROS

```
COMMON/NXCROS/CNX(LNNM,42)
REAL CNX
```

Definitions:

- CNX is the field containing all cross sections $\sigma_{n,x}(E_{n_i})$ for one nucleus A. It is just handling with the data of one nucleus at a time, and it is refilled for each next nucleus A in the REAC-ECN-5 file. The (n, x) cross sections are stored in field indices corresponding to the (n, x) reaction type. For further information look into the description of the subroutine PCGCNX.

Access:

The common block NXCROS is used by the following subroutines:
PCGCNX, PCPRES, PCRESA.

3.2.15. Common block STOPPS

```
COMMON/STOPPS/SPP(LXGR,LELE),SPD(LXGR,LELE),SPA(LXGR,LELE),
&          SPT(LXGR,LELE),SPH(LXGR,LELE),
&          IELP(LELE),IELD(LELE),IELA(LELE),
&          IELT(LELE),IELH(LELE)
REAL      SPP,SPD,SPA,SPT,SPH
INTEGER   IELP,IELD,IELA,IELT,IELH
```

Definitions:

- SPP contains quantities $\Delta R_p(E_{p_k})$ (cm) which refer to the differential thickness of the surrounding material corresponding to the 1 MeV energy loss of protons with the starting energy E_{p_k} .
- SPD,SPA,SPT and SPH contain the corresponding quantities as above, but now for d, α, t and ${}^3\text{He}$ particle, respectively.
- IELP contains the element identifiers of the surrounding material in the case that protons are passing through. The form of the element identifiers is EEEIIM.
- IELD, IELA, IELT and IELH contain element identifiers similar to IELP, but now for d, α, t and ${}^3\text{He}$ particle, respectively.

Access:

The common block STOPPS is used by the following subroutines:
PCGSTP, PCPRES, PCREAD.

3.2.16. Common block SPECTA

```
COMMON/SPECTA/NFLUX(LNNM)
&          SUMLET,
&          IFLUXC
REAL      NFLUX,SUMLET
INTEGER  IFLUXC
```

Definitions:

- **NFLUX** contains the initial neutron flux $\Phi_n(E_{n_i})$.
- **SUMLET** is the integral of the above initial neutron flux $\Phi_n(E_{n_i})$.
- **IFLUXC** contains the group structure of the initial neutron flux $\Phi_n(E_{n_i})$. In the 1.0 version of the PCROSS only the 175 group structure of the REAC-ECN-5 file is supported.

Access:

The common block SPECTA is used by the following subroutines:
PCCALC, PCCALS, PCRDU5, PCREAD.

3.2.17. Common block XNCROS

```
COMMON/XNCROS/XNP(LXGR,LISO),XND(LXGR,LISO),XNA(LXGR,LISO),
&          XNT(LXGR,LISO),XNH(LXGR,LISO),
&          X2P(LXGR,LISO),X2D(LXGR,LISO),X2A(LXGR,LISO),
&          X2T(LXGR,LISO),X2H(LXGR,LISO),
&          IXCP(LISO),IXCD(LISO),IXCA(LISO),
&          IXCT(LISO),IXCH(LISO),
&          IX2P(LISO),IX2D(LISO),IX2A(LISO),
&          IX2T(LISO),IX2H(LISO)
REAL      XNP,XND,XNA,XNT,XNH,X2P,X2D,X2A,X2T,X2H
INTEGER  IXCP,IXCD,IXCA,IXCT,IXCH,IX2P,IX2D,IX2A,IX2T,IX2H
```

Definitions:

- **XNP** contains the (p,n) cross section $\sigma_{p,C}(E_{pk})$ and it stands for the production cross section of the nucleus C via the sequential reaction $\bar{A}(p,n)C$.
- **XND**, **XNA**, **XNT**, **XNH** contain similar cross sections as above for reactions $\bar{A}(x,n)C$, where x refers to d, α , t and ${}^3\text{He}$ particle, respectively.
- **X2P**, **X2D**, **X2A**, **X2T** and **X2H** contain (x,2n) cross sections in the same way as described above. However, only (d, 2n) and (t, 2n) cross sections are currently available from the library KFKXN.
- **IXCP** contains the identifier of the isotopes \bar{A} for the proton reaction $\bar{A}(p,n)C$. The form of the isotope identifier is EEEIIM.
- **IXCD**, **IXCA**, **IXCT**, **IXCH** and **IX2P**, **IX2D**, **IX2A**, **IX2T**, **IX2H** contain the isotope identifiers similar as in IXCP. The identifiers IXCx refer to XNx cross section fields and identifiers IX2x refer to X2x cross section fields.

Access:

The common block **XNCROS** is used by the following subroutines:
PCGCXN, PCLOOP, PCREAD.

4. Subroutines

In this section the purpose of the subroutines is described. A shorter description of the subroutines can be also found in Ref.[4]. We remind the reader of Fig.2 where it is sketched out how the complete program is fitting into the inventory calculation chain of FISPACT.

4.1. Subroutine PCHEAD

This subroutine prints an output header on output unit number 6.

Common blocks used:

No common block is used.

4.2. Subroutine PCINIT

This subroutine contains dummy OPEN statements. The OPEN statements are depending on the operation system (OS). The dummy OPEN statements implemented are used for the OS named MVS used for an IBM 3090 mainframe with a preallocation system. The input units needed to be opened are LIN1 - LIN7, LIN10 - LIN14 and LIN20 - LIN26. The output units needed to be opened are LOUT and LRES.

The user is forced to make changes to all OPEN statements whenever he uses other OS like VMS, UNIX or DOS. Furthermore, a BLOCK DATA statement is appended to this subroutine which initializes the common blocks mentioned below.

Common blocks used:

DFLUXS, ECONST, IDENTI, PNames, NEUTRN.

4.3. Subroutine PCREAD

It reads files from the input units opened either by PCINIT or the Operation System. These are the files of the libraries KFKSTOP and KFKXN that are stored in the common blocks /STOPPS/ and /XNCROS/. Furthermore, the initial neutron spectrum and the

FISPACT isotope identifier are read-in. The data are stored into the common blocks listed below.

Common blocks used:

IFISDI, SPECTA, STOPPS, XNCROS.

4.4. Subroutine PCRDU5

This subroutine reads the Input Data Cards from the default input unit 5. The use of the Input Data Cards is explained in detail in the user manual to the code PCROSS [4].

Common blocks used:

LSTEER, P NAMES, SPECTA.

4.5. Subroutine PCLOOP

The subroutine PCLOOP is built-in to call for major loops in order to calculate "pseudo" cross sections.

The first major loop calls for the subroutines PCGCNX and PCGCPS to get all the cross sections $\sigma_{n,x}(E_{n_i})$ and the normalized charged particle spectra $f_{n,x}(E_{n_i}, E_{x_j})$ for one isotope. Whenever the loop detects that an isotope belongs to the chosen initial composition, the subroutines PCPRES and PCCALS are called to compute the partial contribution to the charged particle flux $\Phi_x(E_{x_k})$.

In the second major loop the charged particle flux $\Phi_x(E_{x_k})$ of the initial material composition is used to compute "pseudo" cross sections for individual isotopes. The various nuclides \bar{A} which shall be taken into account are listed in the field CALVEC of the common block /IDENTI/. Here, the reaction for a given "pseudo" cross section is developed and whenever the "pseudo" cross section is determined, the reaction is stored together with the value of the "pseudo" cross section. This part of the subroutine PCLOOP is steered by the Input Data Cards, see Ref. [4].

Common blocks used:

CPSCDC, CVALUE, ECONST, IDENTI, IFISDI, LSTEER, PCIDIS, PCCTRL, PCSTOP, P NAMES, XNCROS.

4.6. Subroutine PCGCNX

It traces (n, x) cross section data from the file REAC-ECN-5 connected to LIN2. For one isotope at a time it reads all available $\sigma_{n,x}(E_{n,i})$ cross sections and stores them in the field CNX of the common block /NXCROS/. The identifier of the target isotope of the cross sections is stored in IDNOW. It will skip the reading when the logical variable LCPSKH is true.

Common blocks used:

LSTEER, NXCROS, PCIDIS, PCCTRL, PCSTOP, P NAMES.

4.7. Subroutine PCGCPS

It traces the normalized charged particle spectrum $f_{n,x}(E_{n,i}, E_{x,j})$ from the file of the KFKSPEC library connected to LIN5. The spectrum is stored in the common block /CPARTS/. It will skip the reading if the logical variable LCPSKP is already true when the subroutine is called.

Whenever the identifiers IDNOW and IDCPAI are identical, the cross sections and the charged particle spectrum are matching together and the subroutine can check whether this isotope is belonging to the initial material composition or not. Whenever the identifiers IDNOW and ICCPAI are not matching together the logical variables LCPSKP or LCPSKH are set true.

Common blocks used:

CPARTS, PCCTRL, PCIDIS, PCSTOP, P NAMES.

4.8. Subroutine PCGECO

This subroutine is called in the first major do loop of PCLOOP. It checks whether a certain isotope is in the FISPACT index list and whether elemental constants of the isotope (natural abundance of the isotope, density of the element and atomic weight) as well as decay data are available. It determines the number of atoms of the isotope in the initial material composition and stores the results in the common block /CVALUE/.

Common blocks used:

CVALUE, ECONST, PCCTRL, PCIDIS.

4.9. Subroutine PCPRES

It sums up (n, x) cross sections from those reaction channels where an outgoing charged particle x is identical. For example, total production cross sections for protons are obtained as $\sigma^{tot}(n, p) = \sigma(n, p) + \sigma(n, np) + 2\sigma(n, 2p)$. The resulting charged particle production cross sections are stored in the common block /CVALUE/.

Furthermore, it is selecting $\Delta R_x(E_{x_k})$ via pointers ISPPNT and normalized charged particle spectrum $f_{n,x}(E_{n_i}, E_{x_j})$ (MeV^{-1}) for the kind of charged particle x for which the partial charged particle flux $\Phi_x(E_{x_k})$ will be calculated in the subroutine PCCALS.

Common blocks used:

CPARTS, CVALUE, IDENTI, NXCROS, PCCTRL, STOPPS.

4.10. Subroutine PCCALS

It calculates the partial charged particle flux $\Phi_x(E_{x_k})$ according to the data found by subroutines PCGCNX and PCGCPS. It adds this portion of the spectrum to the charged particle flux calculated previously into the field SUMCPS, so that the charged particle flux referring to the complete initial material composition is created.

This is done separately for each type of charged particles so that altogether 5 different charged particle fluxes are obtained. The final charged particle fluxes are stored in the common block /CVALUE/.

Common blocks used:

CVALUE, DFLUXS, IDENTI, SPECTA.

4.11. Subroutine PCGCXN

It traces the fields in the common block /XNCROS/ to get the position of the $\bar{A}(x, n)C$ cross sections $\sigma_{x,C}(E_{p_k})$ for all kinds of charged particle x and a given nucleus

\bar{A} . The pointers are stored in the field IXCPNT. The nucleus \bar{A} is stored in the field CALVEC and the pointer ICALPT is pointing on it.

Common blocks used:

IDENTI, PCCTRL, XNCROS.

4.12. Subroutine PCGSTP

It selects the differential ranges $\Delta R_x(E_{x_k})$ for all kinds of charged particles x , in a given element or, if necessary, it calculates the weighted differential ranges for a given elementary composition in a particular alloy. The subroutine makes use of the common block STOPPS. The pointers are stored in the field ISPPNT.

Common blocks used:

IDENTI, LSTEER, PCCTRL, PCIDIS, P NAMES, STOPPS.

4.13. Subroutine PCCALC

It calculates the "pseudo" cross section for a certain reaction on a certain isotope. It is called in the case that the subroutine PCLOOP has successfully checked that all data needed for the calculation are available.

Common blocks used:

CVALUE, IDENTI, SPECTA.

4.14. Subroutines PCRESA, PCRESP, PCRESC

These three subroutines, PCRESA, PCRESP and PCRESC are cleaning up several common blocks after the subroutine PCCALC has been called.

PCRESA performs a reset to the following common blocks:

IDENTI, XNCROS, PCCTRL, PCIDIS.

PCRESP performs a reset to the following common block:

CVALUE.

PCRESC performs a reset to the following common blocks:

CVALUE, PCCTRL.

4.15. Subroutine PCMERG

It merges all calculated "pseudo" cross sections together with the pre-calculated FISPACT "collapsed" cross sections into one file on the unit LRES. In addition the "pseudo" cross sections are written to the file on unit LOUT. The subroutine is sensitive to the order of initial isotopes which is required by the inventory code FISPACT. This process is steered by Input Data Cards.

It traces over the ICOUNT number of calculated "pseudo" cross sections stored in the common block /CPSCDC/. Whenever the subroutine detects that the identifiers of the nuclei \bar{A} and C appear at least twice (say, for (p,n) and (d,2n) reactions), the corresponding "pseudo" cross sections will be added before merging them into the final cross section file. A more detailed output will be given into the default FORTRAN output unit number 6.

For more details concerning the file containing pre-calculated "collapsed" cross sections see Ref.[6].

Common blocks used:

CPSCDC, LSTEER, P NAMES.

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Figure 1: Flow chart of inventory calculation with FISPACT only

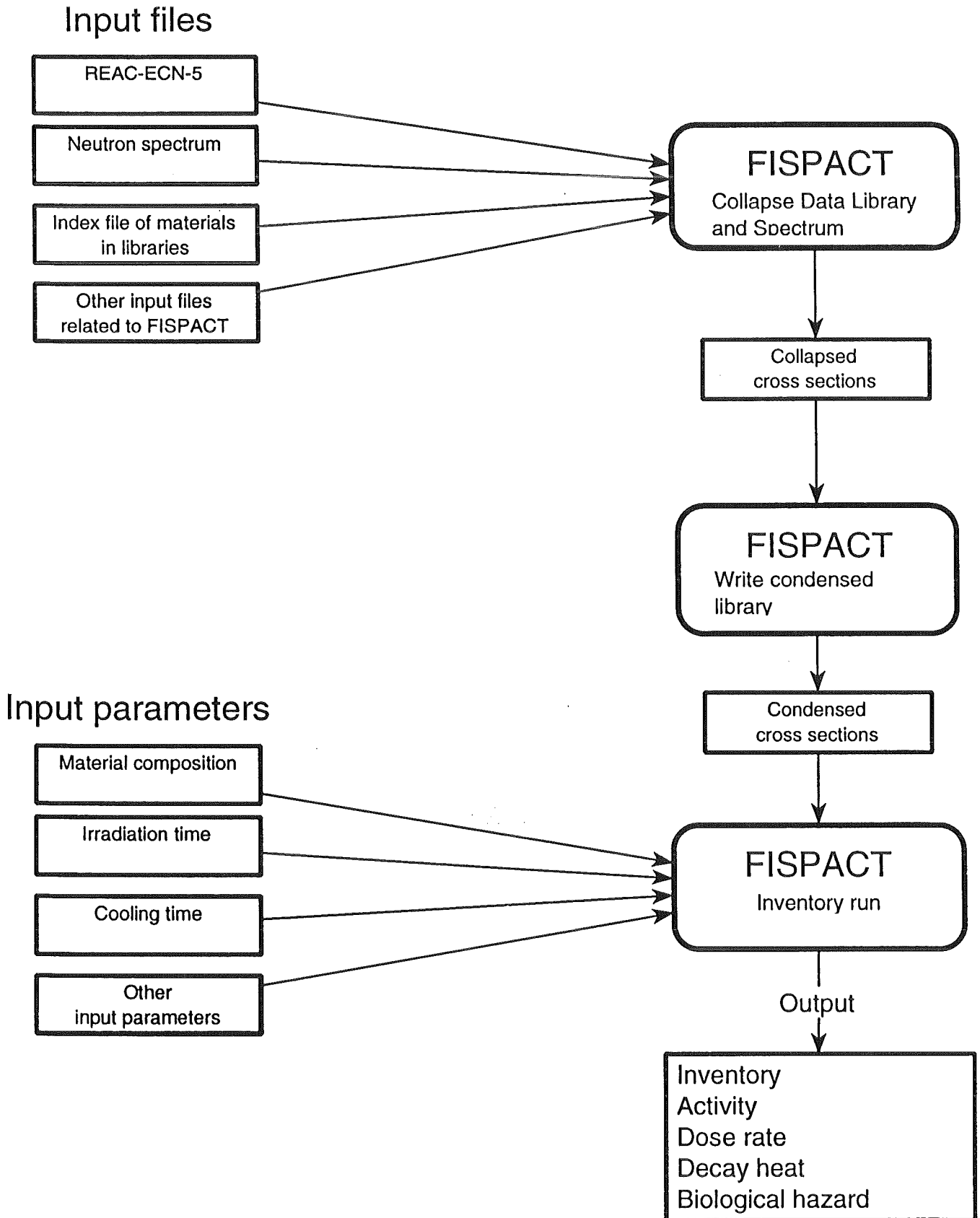


Figure 2: Flow chart of inventory calculation with PCROSS and FISPACT

